Bread leavening and baking: a modelling challenge

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DIPARTIMENTO MATEMATICA

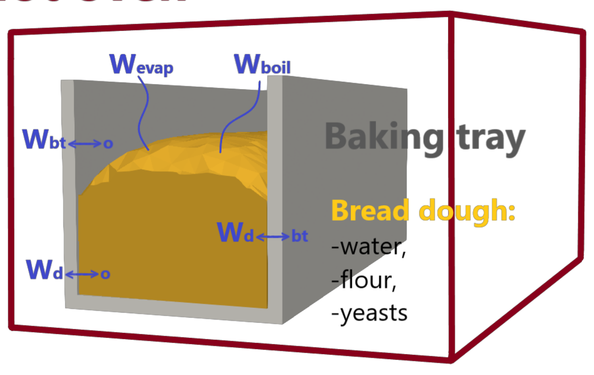
Motivations

The main idea of the project is to construct the **digital twin** of the bread baking to monitor the energy consumption of the process. For this purpose we have to perform these tasks:

1. Construct a **numerical model** which simulates the physical process governed by differential equations;
2. Define an **inverse problem**, based on the previous numerical model, to set parameters;
3. Define an **algorithm of energy estimation** to underline how much power is wasted.

The numerical model

Hot oven



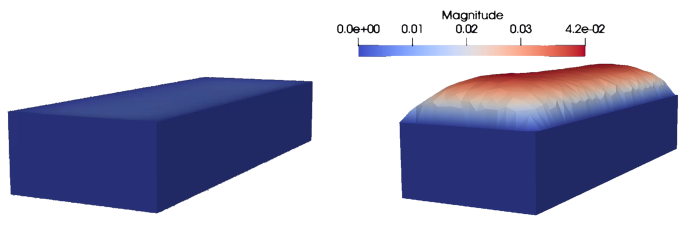
The case of our study is a bread dough made of a certain quantity of water, flour and yeasts, contained in a steel baking tray which, during cooking, is put in a hot oven.
The partial differential equations that describe the heat exchanges and the presence of moisture, yeast and carbon dioxide are coupled with the quasi-static evolution of the growing elastic dough.

The differential equations involved

The paste is treated as a hyperelastic material so, under the action of the gravity, it has an elastic behavior and it is subject to a first small deformation due to its weight then, thanks to the yeasts presence, there will be a positive volume expansion,

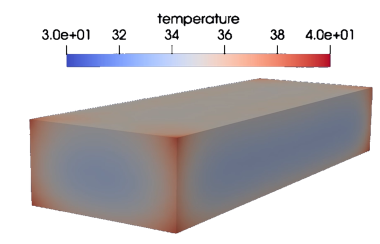
$$E(u) = \int_\Omega \frac{\mu}{2}(C - 3\sqrt[3]{J_{ref}^2}) + \frac{\lambda}{2}(\log(J) - \log(J_{ref}))^2 dX - \int_\Omega B \cdot u \, dX \tag{1}$$

The elasticity equation is $\delta E(u) = 0$.



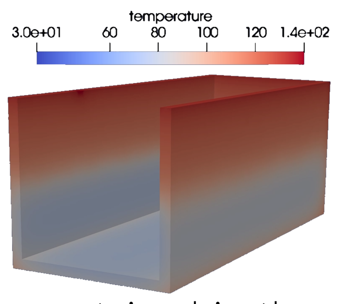
During the cooking process the temperature of the dough changes following the heat equation, where the boundary conditions describe the energy interactions between the paste with the tray or the air in the oven, and considering the heat lost for the evaporation or the boil phenomena,

$$\int_\Omega \rho \, c_p \, J \frac{\partial \theta}{\partial t} \tilde{\theta} dX + \int_\Omega (k \, J \, C^{-1} \nabla_X \theta) \cdot (\nabla_X \tilde{\theta}) dX = \\ = W_{o \longrightarrow d} + W_{bt \longrightarrow d} + W_{loss} \, . \tag{2}$$



The temperature of the steel baking tray also evolves when we put into the oven,

$$\int_{\Omega_{bt}} \rho_{bt} \, c_{bt} \frac{\partial \theta_{bt}}{\partial t} \tilde{\theta}_{bt} dX + \int_{\Omega_{bt}} (k_{bt} \nabla_X \theta_{bt}) \cdot (\nabla_X \tilde{\theta}_{bt}) dX = \\ = W_{o \longrightarrow bt} + W_{d \longrightarrow bt} \, . \tag{3}$$



Due to the evaporation and the boiling phenomena the water density, contained in the paste, decreases and diffuses,

$$\int_\Omega J \, \frac{\partial \rho_m}{\partial t} \, \tilde{\rho}_m dX + \int_\Omega (\beta \, J \, C^{-1} \nabla_X \rho_m) \cdot (\nabla_X \tilde{\rho}_m) dX = M_{loss} \, . \tag{4}$$

The concentration of yeast, uniformly distributed in the paste, evolves in time, according to temperature reached by the loaf,

$$\begin{cases} \frac{d}{dt} Y = K_y(\theta) Y, \\ Y(0) = Y_0. \end{cases} \implies \quad Y(t) = \exp(\, K_y(\theta) \, t) Y_0. \tag{5}$$

The metabolism of the yeasts implies a CO_2 production and diffusion in the paste as follows

$$\int_\Omega J \, \frac{\partial D}{\partial t} \, \tilde{D} dX + \int_\Omega (\beta_{co2} \, J \, C^{-1} \nabla_X D) \cdot (\nabla_X \tilde{D}) dX = \int_\Omega f(\theta) \, Y \, \tilde{D} dX. \tag{6}$$

The rate of CO_2 involves a volume expansion because of the proving of the bread under specific conditions on temperature and moisture. The elastic stiffness are updated according to the CO_2 quantity, so the elasticity equation is rerun to obtain the volume expansion which simulates the leavening.

Paving the way for inverse problem

The results of the simulation provide a starting point for setting up suitable parameter identification.

We want to estimate the CO_2 production during leavening, thus we apply a methodology which simulates a carbon dioxide bubble with a fictitious source term added to the equation [1].

This allows to reformulate the inverse problem from a (nonlinear) domain shape estimation problem [3] to a (linear) heat source estimation one [2].

Replacing voids with fictitious sources in heat conduction problems

Let us consider two open and simply connected bounded domains Ω_B and Ω_C in $\mathbb{R}^n$ such that $\Omega_D := \Omega_B \setminus \overline{\Omega_C}$, where Ω_C represents a cavity within the body Ω_B and the heat conduction problem, stated on Ω_D, for the temperature field $T : \Omega_D \times [0, \tau] \to \mathbb{R}$.

$$\begin{cases} \rho c \partial_t T = k \Delta T & \text{on } \Omega_D \times [0, \tau], \\ k \nabla T \cdot n = g & \text{on } \Omega_B \times [0, \tau], \\ k \nabla T \cdot n = 0 & \text{on } \Omega_C \times [0, \tau], \\ T(0, \cdot) = T_0(\cdot) & \text{on } \Omega_D. \end{cases} \tag{7}$$

- the final time $\tau > 0$
- the mass density $\rho > 0$
- the specific heat $c > 0$
- the thermal conductivity $k > 0$
- the unit outer normal n to Ω_D
- the heat flux on the external boundary g
- the initial temperature field T_0

We show the equivalence of (7) with a second differential problem, stated on the filled domain Ω_B, for the temperature field $\tilde{T} : \Omega_B \times [0, \tau] \to \mathbb{R}$.

$$\begin{cases} \rho c \partial_t \tilde{T} = k \Delta \tilde{T} + f & \text{on } \Omega_B \times [0, \tau], \\ k \nabla \tilde{T} \cdot n = g & \text{on } \Omega_B \times [0, \tau], \\ \tilde{T}(0, \cdot) = \tilde{T}_0(\cdot) & \text{on } \Omega_B. \end{cases} \tag{8}$$

- $\tilde{T} = T$ on $\Omega_D \times [0, \tau]$
- $\tilde{T}_0 = T_0$ on Ω_D

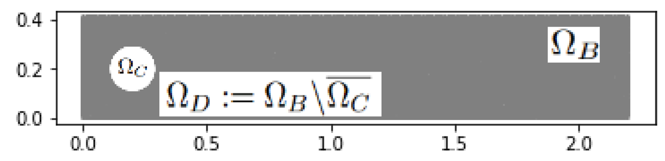
Theorem

Given a solution T of the differential problem (7) with smooth boundary data g and initial condition T_0, there exists a fictitious source field $f : \Omega_B \times [0, \tau] \to \mathbb{R}$ such that:

(i) *the solution $\tilde{T}$ of the differential problem (8) coincides with T on the domain of the latter;*
(ii) *$f = 0$ in the physical domain $\Omega_D \times [0, \tau]$.*

A numerical example

We take the filled domain $\Omega_B \subset \mathbb{R}^2$ as a rectangle and the cavity Ω_C as a circle.



- To emulate a void with a fictitious heat source, we look for an extension of the temperature field within the region corresponding to the void, matching the boundary conditions for temperature and heat flux. This extension is not unique and leads to different estimation scenarios [4], but we can select one as the solution of the following problem:

$$\begin{cases} -\Delta(\tilde{T} - \varepsilon^2 \Delta \tilde{T}) = 0 & \text{on } \Omega_C, \\ \tilde{T} = T & \text{on } \Omega_C, \\ \nabla \tilde{T} \cdot n = 0 & \text{on } \Omega_C. \end{cases} \tag{9}$$

- The fictitious heat source, computed by applying the heat operator to the temperature extension, has compact support within the region corresponding to the cavity, allowing us to estimate the geometry of the void;

$$f = \rho c_t \tilde{T} - k \Delta \tilde{T} \qquad \text{on } \Omega_C. \tag{10}$$

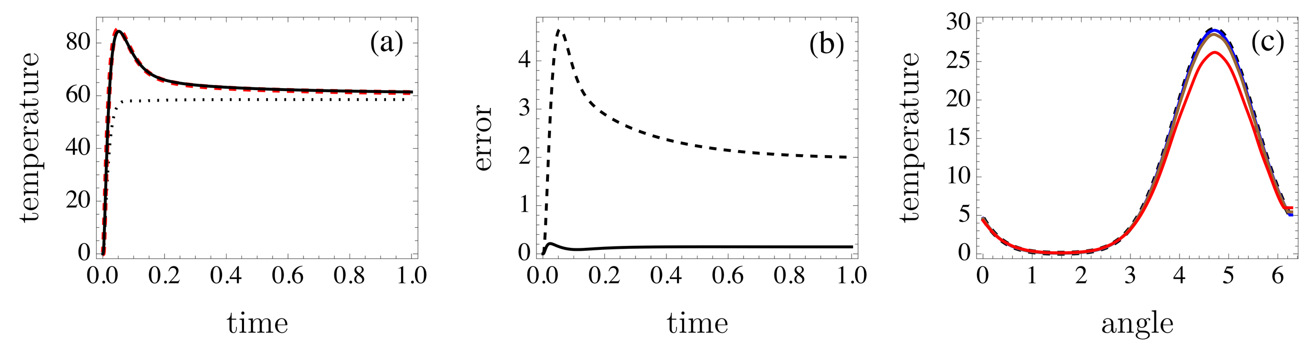


Figure 1. The source term added on the filled domain well simulates the void. (a) The physical temperature evolution at one point on the cavity boundary (red dashed line) is well captured by the solution of the problem with a fictitious force (black solid line), whereas the heat equation on the filled domain and without source term (dotted line) gives a very different prediction. (b) The global error given by the L^2-norm of the difference, on the physical domain, between the physical temperature and the one obtained with the fictitious force (solid line) is much lower than what would be predicted (dashed curve) using a filled domain and without the fictitious source. (c) The grid refinement is crucial to obtain a good approximation of the datum at the cavity boundary. Here the comparison between boundary data obtained by interpolation (black dashed line) and its reconstruction with Fourier series expansions as the number of mesh nodes on the cavity varies: $40, 80, 160$ nodes (red, brown, blue line respectively).

Algebraic reconstruction of source term

Mathematical results about inverse heat transfer problems ensure that, under suitable hypotheses (for example if it is known that the source expression has separable variables), it is possible to uniquely reconstruct both the temperature evolution and the source term for given time-dependent boundary data (see theorems 6.1, 6.2 and 6.3 in [2]).

The source obtained in our example as solution of (9) has no separable variables in the way required by the cited theorems. To deal with generic situations, we must therefore introduce a numerical estimator that should infer the fictitious heat sources from a restricted set of available data. More precisely, we point toward a model-based estimator, where the model is given by the equations (8) through the algebraic inversion of their discretization in space an time.

Here we study the behavior of this algebraic inversion of the model with respect to the obtainable degree of knowledge about the temperature field values inside the domain.

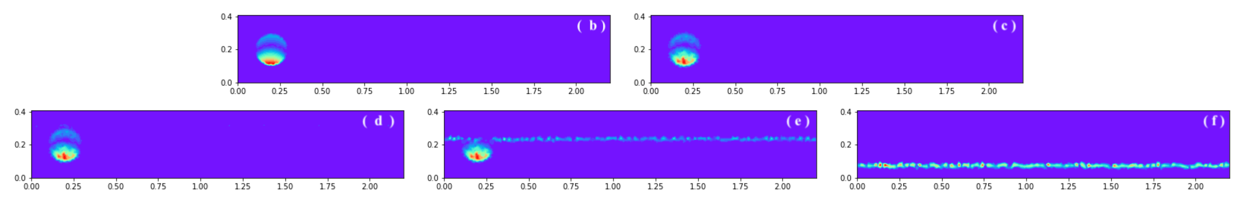


Figure 2. The absolute value of the fictitious source term $|f(t, r, \theta)|$ (b) and its algebraic reconstruction with the sparsity constraint in different conditions as a rainbow color map (max value= red, min value=blue): when all temperatures on Ω_B are known (c), when all temperatures on Ω_B with $y \leq 0.32$ are known (d), when all temperatures on Ω_B with $y \leq 0.24$ are known (e), when all temperatures on Ω_B with $y \leq 0.08$ are known (f).

Future work

Surrogate model

The numerical model is the foundation for a **surrogate/reduced modeling** that can bring the simulations to run online with the real process, a main target of digital twins for Industry 4.0.

- Mimics the behavior of the simulation model as closely as possible;
- Is computationally cheaper to evaluate;
- Needs few data as input.

Inverse problem

Our inverse problem becomes to estimate the fictitious heat source f in (8).

Since the relation between heat source and temperature field is linear, we can express the source field as a linear state space embedded with the temperature state space of the heat equation, and solve it using an efficient recursive formulation of linear least squares estimation of the state vector, i.e. the Kalman Filter, using the measurements taken at the accessible border.

References

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